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TRANSFERS IN POROUS MEDIA

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ABSTRACT

Modelling heat transfer in porous media requires to take into account multiple-scale aspects inherent to porous media structures. Several methodologies have been developed to upscale the equations at a lower-scale and to obtain upper-scale models as it is outlined in a brief review based on a simple heat conduction example proposed in the first part of this paper. The more general and classical problem of heat transfer in porous media is reviewed in this paper with the emphasis on the fact that different behaviours and hence different models emerge at a given macro-scale, depending on the interplay of the various characteristic times and lengths characterizing the problem. Various classes of models are discussed and their relationships outlined. Extensions to more complicated problems of heat transfer in porous media are discussed: coupling with mass diffusion, effect of heat sources, radiation, boiling, etc.

KEY WORDS: Porous media, Multiphase, Upscaling methods

1. INTRODUCTION

Heat transfer in porous media is central in many applications involving industrial devices (chemical engineering, heat exchangers, nuclear reactor, etc...) as well as complex geological formations (in situ combustion and pyrolysis, geothermal sites, etc...). As a consequence, such heat transfer problems are often characterized by highly non-linear couplings with many different scales involved. The most common multi-scale feature is illustrated Fig. 1, which represent a typical porous medium two-scale description. The lower-scale is the pore-scale where phases are differentiated, here a β -phase flowing in a solid structure made of a σ -phase, with pore-scale characteristic lengths l_β and l_σ . The upper-scale or macro-scale calls for an effective representation characterized by variations of the variables at a scale L . To be applicable, such a macro-scale representation requires the validity of a separation of scale assumption implying $l_\beta, l_\sigma \ll r_0 \ll L$ where r_0 is some intermediated scale at which macro-scale variables are defined (this scale is related to the classical discussion about the existence of a Representative Elementary Volume [9, 46]). In the sequel of this presentation, we will assume that all scales involved are nicely separated, but the reader must not forget that this does not happen all the time. If L is too close to l , direct numerical simulation or meso-scale approaches, such as network modelling [32], must be used. Another class of porous media which will not be considered in this paper calls also for specific approaches: those with a fractal structure over a large range of scales ([85]).

In the above paragraph, we have emphasized the need for macro-scale models when dealing with practical applications. Of course, one may introduce ad hoc or heuristic models, and, as a matter of fact, this is the case for many of the classical macro-scale models used in the engineering practice. However, it is often more reliable to have at its disposal a comprehensive framework that links the known pore-scale physics to the associated

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macro-scale theory. Not only this provides a strong basis for developing correct (physically speaking) models, but it also offers a guidance for developing new, original models for surging problems. Because of the problem complexity, mainly due to the multi-scale aspects outlined above, there is not a single route from one pore-scale problem to a macro-scale model. Indeed, two major issues must be addressed:

- Given the interplay between the different mechanisms and the potential contrast of transport properties (such as diffusivities for instance), several behaviours may be observed requiring specific macro-scale models. This is the case with the discussion in Sec. 3 about non-equilibrium and equilibrium models,
- Similarly, it is not surprising to find that many different methods have been designed to deal with the upscaling aspects.

This paper offers a *review* of these two problems. The first section proposes a brief overview of the different available upscaling techniques. Next, the potential for different macro-scale models will be illustrated for the classical porous medium heat transfer problem. Finally, indications will be given on open or modern problems which are the subject of current research in the area of heat transfer in porous media. Of course, the format of this paper does not allow for writing an encyclopedia, nor a thorough comprehensive review. It is modestly expected that keys will be provided for understanding what it at stake when working on such upscaling problems.

2. UPSCALING METHODOLOGIES: A BRIEF OVERVIEW

To illustrate the problem, let us start with a simple, steady-state heat transfer problem over a medium with a l -scale heterogeneous but continuous thermal conductivity, $\mathbf{k}(\mathbf{x})$. The typical pore-scale equation would be written as

$$\nabla \cdot (\mathbf{k}(\mathbf{x}) \cdot \nabla T) = 0 \quad (1)$$

This equation is also equivalent, mathematically speaking, to the problem of a Darcy flow in a heterogeneous porous medium or to a classical mass diffusion problem. Therefore, some of the cited papers in the following sections are in fact connected to these latter problems and not heat transfer. We will not stress that meaningless difference.

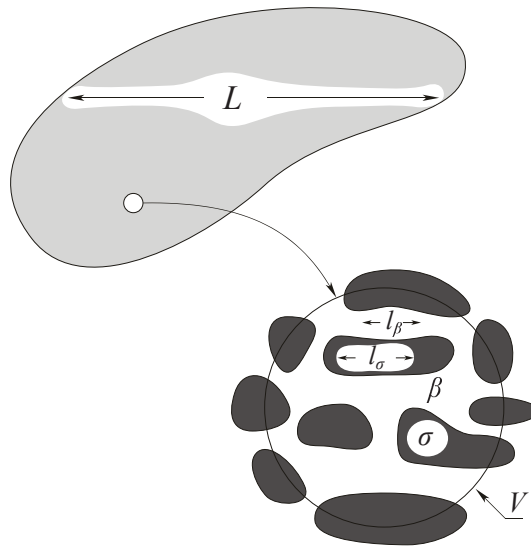


Fig. 1 Multiple-scale description of a porous medium.

2.1 Obtaining a macro-scale theory through volume averaging

How to define macro-scale variables and how to obtain macro-scale equations? Macro-scale variables are in some broad sense regularized fields of the micro-scale fields. This is not surprising that the idea of regularization through some spatial convolution was originally proposed as a designated tool to achieve this task [57, 59, 92, 99]. In this framework, we would define the macro-scale temperature field by

$$\langle T \rangle(\mathbf{x}, t) = \frac{1}{V} \int_{\mathbf{r} \in \mathcal{V}(\mathbf{x})} T(\mathbf{r}) dV_r \quad (2)$$

where $\mathcal{V}(\mathbf{x})$ is a volume centred at \mathbf{x} and of volume V . The regularization process through spatial averaging may require special attention if used with simple kernel functions such as the one involved in Eq. (2). This point is not discussed in this paper and we refer the reader to [57, 59, 63] and the series of paper [76–80] for a better understanding of the problem. A macro-scale equation could be obtained from averaging of the pore-scale equation, and this would lead to

$$\nabla \cdot \langle \mathbf{k}(\mathbf{x}) \cdot \nabla T \rangle = 0 \quad (3)$$

which cannot be readily put under a closed form, i.e., an equation for T^* with some effective property. A work-flow has been proposed to solve this problem and that makes use of the following steps:

Step 1: define temperature deviation

$$T = \langle T \rangle + \tilde{T} \quad (4)$$

Step 2: develop averaged equation

$$\nabla \cdot \langle \mathbf{k}(\mathbf{x}) \cdot (\nabla \langle T \rangle + \nabla \tilde{T}) \rangle = 0 \quad (5)$$

Step 3: obtain micro-scale governing equation for the deviation

$$\nabla \cdot (\mathbf{k}(\mathbf{x}) \cdot \nabla \tilde{T}) = -\nabla \cdot (\mathbf{k}(\mathbf{x}) \cdot \nabla \langle T \rangle) \quad (6)$$

Step 4: closure, i.e., solve in an approximate manner (using approximations based on the separation of scales) the coupled micro and macro-scale problem

$$\tilde{T} = \mathbf{b} \cdot \nabla \langle T \rangle + \dots \quad (7)$$

where the mapping vector \mathbf{b} is determined by

$$\nabla \cdot (\mathbf{k} \cdot \nabla \mathbf{b}) = -\nabla \cdot \tilde{\mathbf{k}} \quad (8)$$

completed by (not discussed in this paper)

$$\langle \mathbf{b} \rangle = 0 \quad ; \quad \mathbf{b}(\mathbf{x} + \mathbf{l}) = \mathbf{b}(\mathbf{x}) \quad i = 1, 2, 3 \quad (9)$$

where the last equation corresponds to periodicity conditions.

Step 5: Obtain a closed form of the macro-scale equation, i.e.,

$$\nabla \cdot (\mathbf{K}_{eff} \cdot \nabla \langle T \rangle) = 0 \quad (10)$$

in which the effective property, here a thermal conductivity tensor, is given by

$$\mathbf{K}_{eff} = \langle \mathbf{k} \cdot (\mathbf{I} + \nabla \mathbf{b}) \rangle \quad (11)$$

The upscaling process provides not only the form of the equation compatible with the assumptions made, but also a way of calculating the effective property through the knowledge of pore-scale characteristics. While in the past such calculations were considered as too cumbersome and impractical, given the poor access to pore-scale characteristic and the computational requirements, this is now becoming more of a routine thanks to bigger computers and tools like CT-scanners [1]. Indeed, several commercial softwares for CT-scan treatment offer tools to compute the most simple effective properties (diffusivity, permeability, ...).

The above work-flow is a schematic presentation for a simple problem. The reader may find a more comprehensive presentation in [104]. Other techniques were devised to interpret the additional terms that appear when balance equations are averaged. For instance, this can be achieved heuristically [10, 92] or in recognition of the physical notions of tortuosity, dispersion terms, etc... Intermediate approaches have been used to interpret microscale numerical simulations and to propose new forms of macroscale equations (e.g. in [47, 67]), which offers, through a less complex closure, a possible way of dealing with complicated coupled problems.

2.2 Other point of views

Homogenization theory

Asymptotic methods have been used in mathematics to study differential operators involving rapidly oscillating coefficients. The development of the homogenization theory for porous media problems follows this idea, with the macro-scale fields defined in the sense of some limit with respect to a small number, ϵ , characteristic of the separation of scale, i.e., $\frac{l}{L}$. This idea can be developed mathematically speaking following different routes. This is beyond the scope of this paper to provide a complete picture, and we will, for simplicity, outline the development using asymptotic developments for periodic domains, as in [4, 4, 7, 12, 34, 35, 61, 86, 87] and many other contributions. One may refer to [94] for the presentation of a different, less restrictive view. Basically, the temperature field will be looked at in terms of a multi-scale expansion involving \mathbf{x} and \mathbf{y} treated as independent variables in the limit $\epsilon \rightarrow 0$ such as

$$T(\mathbf{x}) = \sum_i T_i \left(\mathbf{x}, \mathbf{y} = \frac{\mathbf{x}}{\epsilon} \right) \epsilon^i \quad (12)$$

where the first term will play the role of the macro-scale variable and the subsequent terms the role of the deviation, like in Eq. (4). The perturbation analysis gives the following results (here we assume that $\mathbf{k}(\mathbf{x}, \mathbf{y}) = \mathbf{k}(\mathbf{y})$).

The ϵ^{-2} term implies $T_0(\mathbf{x}, \mathbf{y}) = T_0(\mathbf{x})$, while the term ϵ^{-1} gives a local (closure) problem such as

$$\nabla_y \cdot (\mathbf{k} \cdot \nabla_y T_1) + \nabla_y \cdot (\mathbf{k} \cdot \nabla_x T_0) = 0 \quad (13)$$

which suggests a solution of the form

$$T_1(\mathbf{x}, \mathbf{y}) = \mathbf{b}(\mathbf{y}) \cdot \nabla_x T_0(\mathbf{x}) \quad (14)$$

with the periodic mapping vector $\mathbf{b}(\mathbf{y})$ obeying

$$\nabla_y \cdot (\mathbf{k} \cdot \nabla_y \mathbf{b}) = -\nabla_y \cdot \mathbf{k} \quad ; \quad \langle \mathbf{b} \rangle = 0 \quad ; \quad \mathbf{b}(\mathbf{x} + \mathbf{l}_i) = \mathbf{b}(\mathbf{x}) \quad i = 1, 2, 3 \quad (15)$$

The ϵ^0 term, after integration over a unit cell, gives the macro-scale equation

$$\nabla_x \cdot (\mathbf{K}_{eff} \cdot \nabla_x T_0) = 0 \quad (16)$$

where the effective thermal conductivity is given by

$$\mathbf{K}_{eff} = \langle \mathbf{k} \cdot (\mathbf{I} + \nabla_y \mathbf{b}) \rangle \quad (17)$$

This is beyond to scope of this paper to give a complete comparison between the two methods. The reader may refer to a preliminary work by [16] and a more thorough analysis by [26]. One sees from the two developments that:

- the operational definition of the macro-scale variables is different, while one may recognize that $\langle T \rangle = \langle \sum_i T_i(\mathbf{x}, \mathbf{y} = \frac{\mathbf{x}}{\epsilon}) \epsilon^i \rangle = T_0$,
- closure is based on a perturbation analysis making use of the separation of scales, through order of estimates analysis or through the manipulation of the "independent" variables (in a limit sense) \mathbf{x} and \mathbf{y} ,
- the macro-scale equation is obtained after averaging the micro-scale equation, taking into account the separation of scales.

Given the fact that both methods solve the same deterministic problem, it is not surprising that the perturbation analysis gives the same "closure" and the same macro-scale equation.

Stochastic method

A non deterministic point of view has been adopted by many scientists, especially in the field of hydrogeology [22, 24, 39, 60]. Because of the complex and more or less disordered heterogeneities found in natural media, the actual porous medium is seen as a particular realization of a stochastic ensemble and, therefore, the macro-scale variable is defined as an expectation, i.e.

$$T^e = E(T) \quad (18)$$

While there is not a direct connection between $T^e = E(T)$ and $\langle T \rangle$, the link between the stochastic point of view and spatial averaging comes from an ergodicity assumption which is most often (but not always [23]!) considered when building the ensemble statistical properties. In this framework, the thermal conductivity in the heat equation becomes a random space function and the heat equation itself is a stochastic PDE. Many different techniques are available to get solutions of the corresponding stochastic problem, and they do not compare necessarily with the methods described above for volume averaging with closure or for the homogenization theory. However, some methods make use of a perturbation analysis in terms of the covariance of k (see [13, 22]), which is reminiscent of the way a "closure" is obtained with the previously introduced two-scale methods. One may refer to [107] for a comparison between a stochastic analysis of the problem of dispersion in [38] and results obtained with the use of a volume averaging theory [73].

A less limited approach in terms of the thermal conductivity variance corresponds to the self-consistent method and the many variants also called effective-medium theories in which the effective conductivity is built from the calculation of the interaction between an inclusion embedded into a homogeneous medium having the effective transport property [22].

While this also can be done through the examination of the closure problems for the method of volume averaging or the homogenization theory, stochastic analysis allows to develop in a quite straightforward manner bounds for the effective thermal conductivity. One easily obtain (see [22], chap. 2) by looking at the expectation for the flow energy that

$$K_H \leq K_{eff} \leq K_A \quad (19)$$

where K_H and K_A are the harmonic mean and arithmetic mean respectively of the pore-scale thermal conductivity. This question of bounds for the effective properties is of a great practical importance. Wiener's bounds [105], as expressed by Eq. 19, are in general too far apart and more narrow bounds, can be developed for *specific classes* of material, see a popular example in [44] or a more thorough discussion in [95].

Variants

The method of volume averaging has triggered many variants. For example, [57, 58] tried to justify Darcy's law using irreversible thermodynamics. The idea that macroscale models should be compatible with the principles of thermodynamics was not new [15, 64, 88], but the coupling with volume averaging produced a specific methodology used by several authors (for instance [45], [11], ...). Such a methodology is also reminiscent of the theory of mixtures (see [17]). While there is not a specific closure, i.e., a deterministic mapping between macro-scale variables and deviations, the structure of the macro-scale models for complex, non-linear coupled systems may be constrained by the method. The method of moments for spatially periodic media, as developed in [18, 50], bears also some resemblance with the two-scale methods discussed in Sec. 2.1 and 2.2.

Many other ideas have been tested and this is beyond the scope of this paper to provide a comprehensive analysis. This short comparison of several methods put the emphasis on:

- the definition of macro-scales variables,
- the way the coupled micro- and macro-scale problems are approximated,
- the existence of an explicit closure, which provides a straightforward way of calculating effective properties from the micro-scale characteristics.

In the next sections, we describe results for more complex heat transfer in porous media problems. Given the format allowed for this contribution, we will not detail the steps for the upscaling developments but rather put the emphasis on several fundamental questions, in particular the question of the *existence of various models* for the same mathematical problem, depending on the flow properties and pore-scale characteristics. An intricate question which is often overlooked and may result in misleading recommendations.

3. THE CLASSICAL HEAT TRANSFER IN POROUS MEDIA PROBLEM

In this section we review the major results corresponding to the classical heat transfer in porous media problem, i.e., diffusion/convection in the fluid saturating the pore space and conduction in the solid phase. We will assume that the flow is laminar and that the fluid density and viscosity are constant. As a consequence, the total mass balance problem and the momentum balance problem can be solved independently. In fact it suffices that the variations over a representative unit cell are small. The one phase flow upscaling problem leads to the classical Darcy's law (see [35, 100]) when the pore-scale Reynolds is small enough. Inertia terms play a role when the pore-scale Reynolds increases and a generalized Forchheimer equation may be used [91, 103, 106]. It has been shown in [53] that this Forchheimer model is relatively robust and accurate. As a consequence of the above decoupling assumption, the macro-scale and micro-scale velocity fields are dealt with independently and are known fields for the pure heat transfer problem described by the following equations.

$$(\rho c_p)_\beta \frac{\partial T_\beta}{\partial t} + (\rho c_p)_\beta \nabla \cdot (\mathbf{v}_\beta T_\beta) = \nabla \cdot (k_\beta \nabla T_\beta) \quad \text{in } V_\beta \quad (20)$$

$$T_\beta = T_\sigma \quad \text{at } A_{\beta\sigma} \quad (21)$$

$$\mathbf{n}_{\beta\sigma} \cdot k_\beta \nabla T_\beta = \mathbf{n}_{\beta\sigma} \cdot k_\sigma \nabla T_\sigma \quad \text{at } A_{\beta\sigma} \quad (22)$$

$$(\rho c_p)_\sigma \frac{\partial T_\sigma}{\partial t} = \nabla \cdot (k_\sigma \nabla T_\sigma) \quad \text{in } V_\sigma \quad (23)$$

The objective of this section is not to give the complete mathematical developments but rather to put the emphasis on the different modelling options that emerge, depending on the assumptions made. Therefore, only major steps that illustrate this discussion are reproduced here, using the framework of the theory of volume

averaging [104] as a mere guideline. Additional literature will be cited to complete the learning process for those interested in the upscaling details.

3.1 The structure of the micro-macro coupled problem

As schematically described in Sec. 2.1, we need to develop the coupled macro-scale and micro-scale equations. We only list below the averaged and deviation equation for the β -phase as well as the boundary conditions at $A_{\beta\sigma}$. Averaging of Eq. 20, making use of the classical averaging theorems (see [59] for a proof using the theory of distribution) given by

$$\langle \nabla \psi_\beta \rangle = \nabla \langle \psi_\beta \rangle + \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \psi_\beta dA \quad ; \quad \langle \nabla \cdot \mathbf{A}_\beta \rangle = \nabla \cdot \langle \mathbf{A}_\beta \rangle + \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot \mathbf{A}_\beta dA \quad (24a)$$

$$\left\langle \frac{\partial \psi_\beta}{\partial t} \right\rangle = \frac{\partial \langle \psi_\beta \rangle}{\partial t} - \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot \mathbf{w}_{\beta\sigma} \psi_\beta dA \quad (24b)$$

leads to

$$\underbrace{\varepsilon_\beta (\rho c_p)_\beta \frac{\partial \langle T_\beta \rangle^\beta}{\partial t}}_{\text{accumulation}} + \underbrace{\varepsilon_\beta (\rho c_p)_\beta \langle \mathbf{v}_\beta \rangle^\beta \cdot \nabla \langle T_\beta \rangle^\beta}_{\text{convection}} = \underbrace{\nabla \cdot \left[k_\beta \left(\varepsilon_\beta \nabla \langle T_\beta \rangle^\beta + \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \tilde{T}_\beta dA \right) \right]}_{\text{conduction/tortuosity}} \quad (25)$$

$$- \underbrace{(\rho c_p)_\beta \nabla \cdot \langle \tilde{\mathbf{v}}_\beta \tilde{T}_\beta \rangle}_{\text{dispersion}} + \underbrace{\frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot k_\beta \nabla T_\beta dA}_{\text{interfacial flux}}$$

where we have emphasized the traditional terms arising when upscaling porous media flows, i.e., dispersion and tortuosity effects and exchange terms. The micro-scale equation may be written as

$$(\rho c_p)_\beta \frac{\partial \tilde{T}_\beta}{\partial t} + (\rho c_p)_\beta \tilde{\mathbf{v}}_\beta \cdot \nabla \langle T_\beta \rangle^\beta + (\rho c_p)_\beta \mathbf{v}_\beta \cdot \nabla \tilde{T}_\beta = \nabla \cdot (k_\beta \nabla \tilde{T}_\beta) \quad (26)$$

$$- \varepsilon_\beta^{-1} \nabla \cdot \left(k_\beta \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \tilde{T}_\beta dA \right) - \varepsilon_\beta^{-1} k_\beta \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot \nabla \tilde{T}_\beta dA$$

Similar equations may be written for the σ -phase. The boundary conditions at $A_{\beta\sigma}$ are given by

$$\tilde{T}_\beta = \tilde{T}_\sigma - \underbrace{(\langle T_\beta \rangle^\beta - \langle T_\sigma \rangle^\sigma)}_{\text{source term}} \quad (27)$$

$$- \mathbf{n}_{\beta\sigma} \cdot k_\beta \nabla \tilde{T}_\beta - \underbrace{\mathbf{n}_{\beta\sigma} \cdot k_\beta \nabla \langle T_\beta \rangle^\beta}_{\text{source term}} = - \mathbf{n}_{\beta\sigma} \cdot k_\sigma \nabla \tilde{T}_\sigma - \underbrace{\mathbf{n}_{\beta\sigma} \cdot k_\sigma \nabla \langle T_\sigma \rangle^\sigma}_{\text{source term}} \quad (28)$$

where we have emphasized the *source terms* that will trigger the development of temperature deviations.

3.2 Various models

This coupled problem for the two macro-scale equations and the two micro-scale equations is characterized by several time and length scales. Depending on the way these different scales are ordered, different approximations may be used leading to different macro-scale models. To make it short, we will consider the time-scales

defined by the following estimates: $\frac{(\rho c_p)_\beta l_\beta^2}{k_\beta}$; $\frac{(\rho c_p)_\sigma l_\sigma^2}{k_\sigma}$; $\frac{\varepsilon_\beta (\rho c_p)_\beta L^2}{K_\beta^*}$; $\frac{\varepsilon_\sigma (\rho c_p)_\sigma L^2}{K_\sigma^*}$, where the characteristic macro-scale diffusivities K_β^* and K_σ^* will be specified a posteriori.

Local equilibrium

Local equilibrium arises when all length-scales are well separated between the macro-scale and the micro-scale and when the pore-scale characteristic times are similar. In particular, we have

$$\left(\frac{(\rho c_p)_\beta l_\beta^2}{k_\beta} \approx \frac{(\rho c_p)_\sigma l_\sigma^2}{k_\sigma} \right) \ll \left(\frac{\varepsilon_\beta (\rho c_p)_\beta L^2}{K_\beta^*} \approx \frac{\varepsilon_\sigma (\rho c_p)_\sigma L^2}{K_\sigma^*} \right) \quad (29)$$

As a consequence, the two macro-scale temperatures are close enough so we can introduce the approximation

$$\langle T_\beta \rangle^\beta = \langle T_\sigma \rangle^\sigma = \langle T \rangle \quad (30)$$

with the total heat for the mixture given by

$$\varepsilon_\beta (\rho c_p)_\beta \langle T_\beta \rangle^\beta + \varepsilon_\sigma (\rho c_p)_\sigma \langle T_\sigma \rangle^\sigma = (\rho c_p)^* \langle T \rangle \quad (31)$$

in which the effective heat capacity is a simple average: $(\rho c_p)^* = \varepsilon_\beta (\rho c_p)_\beta + \varepsilon_\sigma (\rho c_p)_\sigma$. Under these circumstances, one may derive a simple closure with the following estimates for the temperature deviations [20]

$$\tilde{T}_\beta = \mathbf{b}_\beta(\mathbf{y}) \cdot \nabla \langle T \rangle(\mathbf{x}, t) + \dots \quad (32a)$$

$$\tilde{T}_\sigma = \mathbf{b}_\sigma(\mathbf{y}) \cdot \nabla \langle T \rangle(\mathbf{x}, t) + \dots \quad (32b)$$

The mapping vectors, \mathbf{b}_β and \mathbf{b}_σ , are given by a steady-state closure problem expressed as

$$(\rho c_p)_\beta \tilde{\mathbf{v}}_\beta + (\rho c_p)_\beta \mathbf{v}_\beta \cdot \nabla \mathbf{b}_\beta = k_\beta \nabla^2 \mathbf{b}_\beta \text{ in } V_\beta \quad (33a)$$

$$\text{B.C.1} \quad -\mathbf{n}_{\beta\sigma} \cdot k_\beta \nabla \mathbf{b}_\beta - \mathbf{n}_{\beta\sigma} k_\beta = -\mathbf{n}_{\beta\sigma} \cdot k_\sigma \nabla \mathbf{b}_\sigma - \mathbf{n}_{\beta\sigma} k_\sigma \text{ at } A_{\beta\sigma} \quad (33b)$$

$$\text{B.C.2} \quad \mathbf{b}_\beta = \mathbf{b}_\sigma \text{ at } A_{\beta\sigma} \quad (33c)$$

$$0 = k_\sigma \nabla^2 \mathbf{b}_\sigma \text{ in } V_\sigma \quad (33d)$$

$$\mathbf{b}_\beta(\mathbf{x} + \mathbf{l}_i) = \mathbf{b}_\beta(\mathbf{x}) ; \mathbf{b}_\sigma(\mathbf{x} + \mathbf{l}_i) = \mathbf{b}_\sigma(\mathbf{x}) \quad i = 1, 2, 3 \quad (33e)$$

$$\langle \mathbf{b}_\beta \rangle = 0 ; \langle \mathbf{b}_\sigma \rangle = 0 \quad (33f)$$

Adding Eq. 26 with its σ -phase counterpart, and substituting the deviations by their expressions Eqs. 32, we obtain the following macro-scale equation

$$(\rho c_p)^* \frac{\partial \langle T \rangle}{\partial t} + \varepsilon_\beta (\rho c_p)_\beta \mathbf{U}_\beta \cdot \nabla \langle T \rangle = \nabla \cdot (\mathbf{K}_{eq}^* \cdot \nabla \langle T \rangle) \quad (34)$$

where the effective thermal conductivity tensor is given by

$$\mathbf{K}_{eq}^* = (\varepsilon_\beta k_\beta + \varepsilon_\sigma k_\sigma) \mathbf{I} + \frac{k_\beta - k_\sigma}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \mathbf{b}_\beta dA - (\rho c_p)_\beta \langle \tilde{\mathbf{v}}_\beta \mathbf{b}_\beta \rangle^\beta \quad (35)$$

It can be estimated experimentally or calculated by solving Eqs. 33 over a representative unit cell of the porous medium, a strategy that becomes more and more popular with the development of CT-scanners or other devices for pore-scale investigation.

Several correlations have been proposed in the literature, see some examples in [48, 49]. The effective diffusivity is very sensitive to the topology and pore-scale physical characteristics, especially when the solid thermal

conductivity is much larger than the fluid conductivity (about two order of magnitude) and when contacts exist between the solid inclusions [69, 90, 109].

Non-equilibrium models

Non-equilibrium models arise when the contrast between the transport properties of the various phases are not well separated. For instance, the diffusivity of the solid phase is much lower than the diffusivity of the fluid phase. In this case, the heat wave goes rapidly through the unit cell and the temperature field relaxes slowly in the solid phase, thus producing a well-known tailing effect. The relaxation process involves many different time-scales (the spectrum is controlled by the eigenvalues of the diffusion problem over the solid phase). This makes the solution of the coupled problem described in Sec. 3.1 non-local in time (memory effects), and perhaps in space (i.e., the solution depends on all time and space values). Indeed, a closure keeping all local time-scales involves a time convolution as has been discussed in [65] for a pure conductive problem and in [28] from a more general perspective. The deviations in this framework are expressed as

$$\tilde{T}_\beta = \mathbf{b}_{\beta\beta} \star \frac{\partial}{\partial t} \nabla \langle T_\beta \rangle^\beta + \mathbf{b}_{\beta\sigma} \star \frac{\partial}{\partial t} \nabla \langle T_\sigma \rangle^\sigma - s_\beta \star \frac{\partial}{\partial t} \left(\langle T_\beta \rangle^\beta - \langle T_\sigma \rangle^\sigma \right) + \dots \quad (36a)$$

$$\tilde{T}_\sigma = \mathbf{b}_{\sigma\beta} \star \frac{\partial}{\partial t} \nabla \langle T_\beta \rangle^\beta + \mathbf{b}_{\sigma\sigma} \star \frac{\partial}{\partial t} \nabla \langle T_\sigma \rangle^\sigma + s_\sigma \star \frac{\partial}{\partial t} \left(\langle T_\sigma \rangle^\sigma - \langle T_\beta \rangle^\beta \right) + \dots \quad (36b)$$

where the mapping variables closure problem are time-dependent. The mapping variables relax more rapidly with time than the macro-scale temperatures and one may seek a steady-state closure under the form [20, 55, 74, 75, 108]

$$\tilde{T}_\beta = \mathbf{b}_{\beta\beta} \cdot \nabla \langle T_\beta \rangle^\beta + \mathbf{b}_{\beta\sigma} \cdot \nabla \langle T_\sigma \rangle^\sigma - s_\beta \left(\langle T_\beta \rangle^\beta - \langle T_\sigma \rangle^\sigma \right) + \dots \quad (37a)$$

$$\tilde{T}_\sigma = \mathbf{b}_{\sigma\beta} \cdot \nabla \langle T_\beta \rangle^\beta + \mathbf{b}_{\sigma\sigma} \cdot \nabla \langle T_\sigma \rangle^\sigma + s_\sigma \left(\langle T_\sigma \rangle^\sigma - \langle T_\beta \rangle^\beta \right) + \dots \quad (37b)$$

where the mapping variables are the limit of the time dependent closure for $t \rightarrow 0$. As an example, the problem for the mapping variables s_β and s_σ is given by

$$(\rho c_p)_\beta \mathbf{v}_\beta \cdot \nabla s_\beta = k_\beta \nabla^2 s_\beta - \varepsilon_\beta^{-1} h_\beta \quad , \text{ in } V_\beta \quad (38a)$$

$$\text{B.C.1. } \mathbf{n}_{\beta\sigma} \cdot k_\beta \nabla s_\beta = \mathbf{n}_{\beta\sigma} \cdot k_\sigma \nabla s_\sigma \quad , \text{ at } A_{\beta\sigma} \quad (38b)$$

$$\text{B.C.2. } s_\beta = 1 + s_\sigma \quad , \text{ at } A_{\beta\sigma} \quad (38c)$$

$$0 = k_\sigma \nabla^2 s_\sigma + \varepsilon_\sigma^{-1} h_\sigma \quad , \text{ in } V_\sigma \quad (38d)$$

$$s_\beta(\mathbf{r} + \mathbf{l}_i) = s_\beta(\mathbf{r}), \quad s_\sigma(\mathbf{r} + \mathbf{l}_i) = s_\sigma(\mathbf{r}) \quad , \quad i = 1, 2, 3 \quad (38e)$$

$$\langle s_\beta \rangle = 0 \quad ; \quad \langle s_\sigma \rangle = 0 h_\beta = \langle \mathbf{n}_{\beta\sigma} \cdot k_\beta \nabla s_\beta \delta_{\beta\sigma} \rangle \quad ; \quad h_\sigma = -\langle \mathbf{n}_{\sigma\beta} \cdot k_\sigma \nabla s_\sigma \delta_{\beta\sigma} \rangle = h_\beta = h_{2eq} \quad (38f)$$

where $\delta_{\beta\sigma}$ is the surface Dirac function on $A_{\beta\sigma}$. It is of a fundamental importance to see that the heat exchange coefficient, h_{2eq} is a result of this integro-differential closure problem and not given a priori. Using this steady-state closure, the macro-scale equations can be written under the form of a generalized two-equation model as

$$\varepsilon_\beta (\rho c_p)_\beta \frac{\partial \langle T_\beta \rangle^\beta}{\partial t} + (\rho c_p)_\beta \langle \mathbf{v}_\beta \rangle \cdot \nabla \langle T_\beta \rangle^\beta - \mathbf{u}_{\beta\beta} \cdot \nabla \langle T_\beta \rangle^\beta - \mathbf{u}_{\beta\sigma} \cdot \nabla \langle T_\sigma \rangle^\sigma = \nabla \cdot \left(\mathbf{K}_{\beta\beta}^* \cdot \nabla \langle T_\beta \rangle^\beta + \mathbf{K}_{\beta\sigma}^* \cdot \nabla \langle T_\sigma \rangle^\sigma \right) - h_{2eq} \left(\langle T_\beta \rangle^\beta - \langle T_\sigma \rangle^\sigma \right) \quad (39a)$$

$$\varepsilon_\sigma (\rho c_p)_\sigma \frac{\partial \langle T_\sigma \rangle^\sigma}{\partial t} - \mathbf{u}_{\sigma\beta} \cdot \nabla \langle T_\beta \rangle^\beta - \mathbf{u}_{\sigma\sigma} \cdot \nabla \langle T_\sigma \rangle^\sigma = \nabla \cdot \left(\mathbf{K}_{\sigma\beta}^* \cdot \nabla \langle T_\beta \rangle^\beta + \mathbf{K}_{\sigma\sigma}^* \cdot \nabla \langle T_\sigma \rangle^\sigma \right) - h_{2eq} \left(\langle T_\sigma \rangle^\sigma - \langle T_\beta \rangle^\beta \right) \quad (39b)$$

where the various effective parameters are obtained from the mapping variables. Making $\langle T_\beta \rangle = \langle T_\sigma \rangle$, one recovers the one equation equilibrium model with

$$\mathbf{K}_{eq}^* = \mathbf{K}_{\beta\beta}^* + \mathbf{K}_{\beta\sigma}^* + \mathbf{K}_{\sigma\beta}^* + \mathbf{K}_{\sigma\sigma}^* \quad (40)$$

Simpler closures may be used depending on the assumptions made on the physical characteristics of the problem [31, 47]. If one drops the additional convective and cross-terms, one recover the traditional two-equation model often used in the literature [40, 89]. The heat exchange coefficient, h_{2eq} , provides one single relaxation time as opposed to the full spectrum discussed in the introduction to this section. Hence, this is not really an intrinsic property of the porous medium and its value depends on the theory used to define it or the type of measurement made. Indeed, several values have been proposed in the literature and we refer the reader to [52] for a more thorough discussion in the case of pure diffusion in a system with a lower diffusivity in the solid. In this case, the proposed values are related to the eigenvalue spectrum of the solid grain diffusive problem in different ways, for instance the first eigenvalue, etc.... The value obtained from the closure problem Eqs. 38 plays a fundamental role, as will be shown in Sec. 3.2, and is related to the harmonic mean of the eigenvalues.

Another problem comes from the periodicity conditions which are often used when solving closure problems (as is the case in Eq. 38e). If one takes, as an analogy of a porous medium problem, heat transfer in a tube (the Graetz problem), such conditions are compatible with the established regime [41]. This produces a smaller impact of the pore-scale Péclet number on the effective heat exchange coefficient as one would estimate by taking into account entrance effects. Taking into account these *entrance* effects would lead to a non-local (in space) analysis. It also contributes to the differences encountered in the literature between the different correlations or estimates of the heat exchange coefficient.

The heat exchange coefficient is also often written as

$$h_{2eq} = a_v h \quad (41)$$

where a_v is the porous medium specific surface and h is an *intrinsic* heat transfer coefficient. This comes from the *supposed* existence of an established film or boundary layer at the pore-scale that can be introduced as a pore-scale boundary condition at $A_{\beta\sigma}$. Indeed, if one assumes that such a boundary condition exists at the pore-scale, one recovers from the upscaling process a two-equation model with an exchange terms written like Eq. 41 [6, 72]. However, it is clear that h should be a result of the upscaling development and not an input. Furthermore, while the appearance of a_v is natural in some upscaling processes, equilibrium adsorption for instance, this is not the case here since the problem giving h_{2eq} involves a diffusive process which will provide cut-off or smoothing for rough or fractal surfaces. Therefore, Eq. 41 is not true in general. This problem is often overlooked in the literature.

The problem of the conditions for the existence of two-temperature regimes has received a lot of attention in the literature [3, 62, 75, 81, 96, 102]. Simple estimates of the various time and length-scales may often be enough in many practical instances to decide whether a non-equilibrium analysis is needed or not, if differences are clear (for instance several order of magnitude). If this is not the case, the matter is a little bit more complex and depends on the geometry and topology of the unit cell [75], the boundary value problem solved [96, 97], the processes involved, for instance natural convection [83], phase change [33, 93], the coupling with reactive transport [36, 70], etc...

Asymptotic behaviour and One-Equation Non-Equilibrium model

It has been shown in [28, 55, 108] that the two equation model can be approximated for a uniform flow asymptotically as $t \rightarrow \infty$ by a classical heat equation

$$\left(\varepsilon_\beta (\rho c_p)_\beta + \varepsilon_\sigma (\rho c_p)_\sigma \right) \frac{\partial \langle T \rangle^{\beta\sigma}}{\partial t} + \varepsilon_\beta (\rho c_p)_\beta \langle \mathbf{v}_\beta \rangle^\beta \cdot \nabla \langle T \rangle^{\beta\sigma} = \nabla \cdot \left(\mathbf{K}_\infty^* \cdot \nabla \langle T \rangle^{\beta\sigma} \right) \quad (42)$$

where

$$\langle T \rangle^{\beta\sigma} = \frac{\left(\epsilon_\beta (\rho c_p)_\beta \langle T_\beta \rangle^\beta + \epsilon_\sigma (\rho c_p)_\sigma \langle T_\sigma \rangle^\sigma \right)}{\left(\epsilon_\beta (\rho c_p)_\beta + \epsilon_\sigma (\rho c_p)_\sigma \right)} \quad (43)$$

is the mixture average temperature and in which \mathbf{K}_∞^* is given by (dropping cross terms)

$$\mathbf{K}_\infty^* = \mathbf{K}_{eq}^* + \frac{1}{h_{2eq}} \frac{\left(\epsilon_\beta (\rho c_p)_\beta \epsilon_\sigma (\rho c_p)_\sigma \right)^2}{\left(\epsilon_\beta (\rho c_p)_\beta + \epsilon_\sigma (\rho c_p)_\sigma \right)^2} \mathbf{U}_\beta \mathbf{U}_\beta \quad (44)$$

We see from this equation that the effective asymptotic thermal dispersion tensor is obviously greater than the local equilibrium value, \mathbf{K}_{eq}^* . One must emphasize that the one-equation non-equilibrium model does not imply that the two-averaged temperature are equal, as discussed in [28, 55]. This merely means that the front spreading tends to mask the lag between the two average temperatures. Another important discovery is that a direct closure can be found based on $\langle T \rangle^{\beta\sigma}$ [27, 66, 73] if one looks at the pore-scale temperature fields through the following decomposition

$$\hat{T}_\beta = T_\beta - \langle T \rangle^{\beta\sigma} \approx \mathbf{b}_\beta^\infty \cdot \nabla \langle T \rangle^{\beta\sigma} ; \hat{T}_\sigma = T_\sigma - \langle T \rangle^{\beta\sigma} \approx \mathbf{b}_\sigma^\infty \cdot \nabla \langle T \rangle^{\beta\sigma} \quad (45)$$

It was proven numerically and analytically [27, 73] that the resulting non-equilibrium one-equation model is similar to Eq. 42 and that the two effective thermal dispersion tensors (two-equation asymptotic behaviour and one-equation non-equilibrium closure) are equal *if* the heat exchange coefficient is the one from the closure provided by Eqs. (38).

Other non-equilibrium one-equation models have been proposed in the literature. For instance, it has been shown in [98] that the two-equation model is equivalent under certain conditions to a dual-phase-lagging heat conduction model. Similarly, it must be noticed that other types of equations may potentially reproduce some of the features of local non-equilibrium situations, for instance equations with fractional derivatives which have already been used for dealing with some problems of dispersion in porous media [84].

Discussion

At this point, we already have at hand several models for the *same* initial pore-scale problem! We refer the reader to [27] (see in particular Fig. 8) for an exploration of their domain of validity for a typical boundary value problem. It is also of a fundamental importance to recognize that transitions between these various models may arise for the same Initial Boundary Value Problem as has been shown in [25]. We reproduce Fig. 2 the averaged temperature fields obtained from direct pore-scale numerical simulations (symbols) over an array of cylinders (injection from the left at constant temperature, Dirichlet condition at the exit) and the one-equation local equilibrium solution. We see that:

- at early stages the solution calls for a local non-equilibrium treatment,
- the asymptotic behaviour is later observed, characterized by a larger thermal conductivity (larger spreading of the thermal plume) than the one-equation equilibrium model,
- because of the boundary condition at the exit, we see that the *conditions revert to local equilibrium!* An error will be made if one would attempt to predict this final temperature field with the asymptotic thermal conductivity value.

From this discussion and the proposed example, we see that one has to be careful when recommending the exclusive use of such and such model, as is sometimes the case in the literature. The proposed model may be

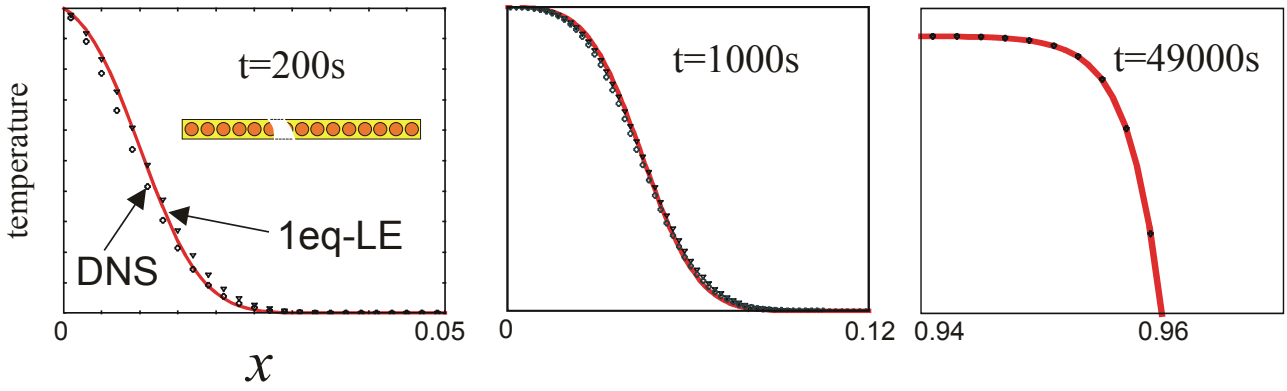


Fig. 2 Transient evolution of macro-scale models (adapted from [25])

acceptable during a time interval and fail after. This is particular true for the asymptotic model since it needs specific conditions to reach the asymptotic limit. Any event that would recondition the temperature fields may lead to its failure. It must be acknowledged that, while it cannot recover all the characteristic times involved in a given thermal process, the two-equation model has the ability to reproduce several regimes since it includes the asymptotic model and the local equilibrium model. This robustness may be used to assess, at the expense of some limited additional complexity, whether the particular process of interest may be affected by local non-equilibrium effects or not.

We already have indicated the limitations of the two-equation model with a single linear or first-order exchange term, i.e., it has only a single characteristic time for describing the fluid-solid temperature relaxation! This drawback may in principle be overcome through the use of the full model with convolution products. However, convolution products are not handy for numerical implementations. Alternate models have been designed to incorporate more characteristic times in the macro-scale equations. One class of models is called multi-rate models, see [42] for an introduction. In general, they may be derived by a splitting of the temperature fields into several sub-phases, either defined by geometrical considerations (for instance grains of big diameters and grains of small diameters) or through a more sophisticated mathematical point of view, for instance using the properties of the eigenvalue spectrum for the diffusion process into the solid phase. This in general leads to N-equation models, which may reproduce the expected several characteristic time behaviour without the inconvenience of convolution products.

A final class of model, called mixed or hybrid models, is based on the following approximation: if the solid phase thermal diffusivity is two order of magnitude or more smaller than the fluid thermal conductivity, i.e., $k_\sigma \sim \epsilon^2 k_\beta$, then Eq. (28) may be approximated by

$$\langle T_\beta \rangle^\beta + \underbrace{\tilde{T}_\beta}_{O(\frac{l_\beta}{L} \langle T_\beta \rangle^\beta)} = T_\sigma \quad \Rightarrow \quad \underbrace{\langle T_\beta \rangle^\beta}_{macro-scale} = \underbrace{T_\sigma}_{micro-scale} \quad (46)$$

The final model combines a micro-scale diffusion equation coupled through Eq. (46) to a macro-scale equation in which the effective thermal dispersion tensor is the one provided by Eqs. (33) with $k_\sigma = 0$. The mixed model works better than the two-equation model in that case, however, it does not work as well as the two-equation model for $k_\sigma \sim \epsilon k_\beta$, as emphasized in [30]. Another type of mixed model may be introduced when sharp thermal fronts are encountered as in [29] in the case of combustion in porous media: they correspond to the use of a micro-scale model in the front matched far from the front with a macro-scale model.

Finally, Fig. 3 summarizes schematically the various models that can be used: direct pore-scale numerical simulation, the various one-equation, 2-equation and N-equation models, as well as mixed models.

4. EXTENSIONS AND OPEN PROBLEMS

In this section, we provide some indications about the extension of the previous models to several classes of problems of general practical importance.

4.1 Heterogeneous and homogeneous heat sources

Homogeneous or heterogeneous heat sources in the energy equations may be uncoupled to heat transfer, for instance in the case of the cooling of nuclear reactor debris beds where the heat source is produced by radioactivity, or may lead to strongly non-linear coupled problems, for instance in the case of smouldering or combustion in porous media. The uncoupled problem has been studied in [82] from an upscaling point of view. The case of local equilibrium can be treated in a very straightforward manner in the case of constant source terms. A constant homogeneous source term, for instance Φ_σ in the σ -phase, does not pose a problem and is simply added as $\varepsilon_\sigma \Phi_\sigma$ to the macro-scale relevant equation in the one-equation or two-equation model. The effect of the heterogeneous source is more tricky and requires an additional closure problem that allows for the distribution of the heat source between the two equations, i.e.,

$$\varepsilon_\beta (\rho c_p)_\beta \frac{\partial \langle T_\beta \rangle^\beta}{\partial t} + (\rho c_p)_\beta \langle \mathbf{v}_\beta \rangle \cdot \nabla \langle T_\beta \rangle^\beta - \mathbf{u}_{\beta\beta} \cdot \nabla \langle T_\beta \rangle^\beta - \mathbf{u}_{\beta\sigma} \cdot \nabla \langle T_\sigma \rangle^\sigma = \nabla \cdot \left(\mathbf{K}_{\beta\beta}^* \cdot \nabla \langle T_\beta \rangle^\beta + \mathbf{K}_{\beta\sigma}^* \cdot \nabla \langle T_\sigma \rangle^\sigma \right) - h_{2eq} \left(\langle T_\beta \rangle^\beta - \langle T_\sigma \rangle^\sigma \right) + a_v \xi \Omega \quad (47a)$$

$$\varepsilon_\sigma (\rho c_p)_\sigma \frac{\partial \langle T_\sigma \rangle^\sigma}{\partial t} - \mathbf{u}_{\sigma\beta} \cdot \nabla \langle T_\beta \rangle^\beta - \mathbf{u}_{\sigma\sigma} \cdot \nabla \langle T_\sigma \rangle^\sigma = \nabla \cdot \left(\mathbf{K}_{\sigma\beta}^* \cdot \nabla \langle T_\beta \rangle^\beta + \mathbf{K}_{\sigma\sigma}^* \cdot \nabla \langle T_\sigma \rangle^\sigma \right) - h_{2eq} \left(\langle T_\sigma \rangle^\sigma - \langle T_\beta \rangle^\beta \right) + a_v (1 - \xi) \Omega + \varepsilon_\sigma \Phi_\sigma \quad (47b)$$

where ξ is the so-called distribution coefficient. Numerical calculations of the distribution coefficient in [82] shows that $\xi \rightarrow 0$ when $k_\sigma/k_\beta \rightarrow \infty$ which leads to the heuristic equation in which all the produced heat is affected to the solid phase [70]. It is interesting to note that this framework has been used to develop a local non-equilibrium model taking into account radiation effects through a generalized radiation transfer equation providing Ω in a coupled manner [54].

The coupling with mass transfer and reaction is often treated with some sort of decoupling [36, 70]. Indeed, if

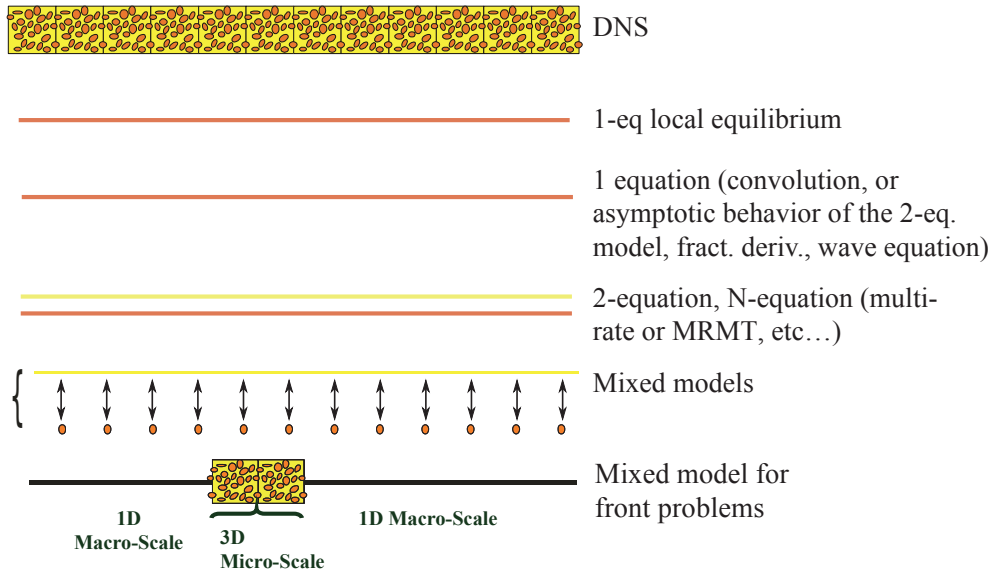


Fig. 3 Multiple-scale description of a porous medium.

we assume that the mass reaction rate is of the form

$$r_\beta = F(c_\beta, T_\beta) = F(\langle c_\beta \rangle^\beta, \langle T_\beta \rangle^\beta) + \frac{\partial F}{\partial c_\beta}(\langle c_\beta \rangle^\beta, \langle T_\beta \rangle^\beta) \tilde{c}_\beta + \frac{\partial F}{\partial T_\beta}(\langle c_\beta \rangle^\beta, \langle T_\beta \rangle^\beta) \tilde{T}_\beta + \dots \quad (48)$$

then neglecting deviations terms based on the estimate $\tilde{T}_\beta = \mathcal{O}\left(\frac{l_\beta}{L} \langle T_\beta \rangle^\beta\right)$ leads to

$$r_\beta = F(c_\beta, T_\beta) = F(\langle c_\beta \rangle^\beta, \langle T_\beta \rangle^\beta) \quad (49)$$

One understands that highly non-linear reaction terms, such as Arrhenius equations, or the potential existence of sharp combustion fronts may require more complicated closures [36] or even call for direct numerical simulations or mixed models [29]. From an upscaling point of view, these problems remain largely open problems.

4.2 Coupling with momentum and mass transport

So far, we have treated the heat equation upscaling problem independently of the mass and momentum transport. This required neglecting density and viscosity variations. We already have emphasized in the above subsection that coupling between the various transport problems may have to be considered.

Often, weak coupling can be treated following the ideas leading to Eq. (49), i.e., density, viscosity, thermal diffusion or mass diffusion are supposed to be constant (to make it simple) over the averaging volume at the intrinsic averaged temperature, pressure, concentration, etc. As a consequence, the closure problems have these averaged values as parameters and the resulting effective parameters will depend non-linearly on $\langle c_\beta \rangle^\beta, \langle T_\beta \rangle^\beta$.

Another class of coupled problems may be treated relatively easily: one-sided coupling. This is the case, for instance, when dealing with thermodiffusion and when Soret effect is only taken into account. Assuming constant fluid and solid characteristics, the thermal upscaling problem may be treated independently of the species transport problem which is defined by

$$\frac{\partial c_\beta}{\partial t} + \nabla \cdot (c_\beta \mathbf{v}_\beta) = \nabla \cdot (D_\beta \nabla c_\beta + D_{T\beta} \nabla T_\beta) \quad (50)$$

$$\text{B.C.1} \quad \mathbf{n}_{\beta\sigma} \cdot (D_\beta \nabla c_\beta + D_{T\beta} \nabla T_\beta) = 0 \quad \text{at } A_{\beta\sigma} \quad (51)$$

Because of this one-side decoupling, the temperature deviations can be estimated from the various closures presented in this paper, i.e., Eqs. (32) or (37). In turn, it can be introduced in the mapping expression for the concentration deviation. For instance, the local equilibrium closure would lead to [25]

$$\tilde{c}_\beta = \mathbf{b}_{C\beta} \cdot \nabla \langle c_\beta \rangle^\beta + \mathbf{b}_{S\beta} \cdot \nabla \langle T \rangle \quad (52)$$

The closure problems for $\mathbf{b}_{C\beta}$ is the classical problem leading to the dispersion tensor [18, 19] while the closure problem for $\mathbf{b}_{S\beta}$ is coupled with the closure problem for \mathbf{b}_β described by Eqs. (33). We have

$$\mathbf{v}_\beta \cdot \nabla \mathbf{b}_{S\beta} = D_\beta \nabla^2 \mathbf{b}_{S\beta} + D_{T\beta} \nabla^2 \mathbf{b}_\beta \quad (53a)$$

$$\text{B.C.} \quad -\mathbf{n}_{\beta\sigma} \cdot (D_\beta \nabla \mathbf{b}_{S\beta} + D_{T\beta} \nabla \mathbf{b}_\beta) = \mathbf{n}_{\beta\sigma} \cdot D_{T\beta} \quad \text{at } A_{\beta\sigma} \quad (53b)$$

$$\mathbf{b}_{S\beta}(\mathbf{r} + \mathbf{l}_i) = \mathbf{b}_{S\beta}(\mathbf{r}), i = 1, 2, 3 \quad \text{and} \quad \langle \mathbf{b}_{S\beta} \rangle^\beta = 0 \quad (53c)$$

and the resulting macro-scale dispersion equation is

$$\frac{\partial \varepsilon_\beta \langle c_\beta \rangle^\beta}{\partial t} + \nabla \cdot (\varepsilon_\beta \langle \mathbf{v}_\beta \rangle^\beta \langle c_\beta \rangle^\beta) = \nabla \cdot (\varepsilon_\beta \mathbf{D}_\beta^* \cdot \nabla \langle c_\beta \rangle^\beta + \varepsilon_\beta \mathbf{D}_{T\beta}^* \cdot \nabla \langle T \rangle) \quad (54)$$

where the effective thermal diffusion tensor is given by

$$\mathbf{D}_{T\beta}^* = D_\beta \left(\frac{1}{V_\beta} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \mathbf{b}_{S\beta} dA \right) + D_{T\beta} \left(\mathbf{I} + \frac{1}{V_\beta} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \mathbf{b}_{T\beta} dA \right) - \langle \tilde{\mathbf{v}}_\beta \mathbf{b}_{S\beta} \rangle^\beta \quad (55)$$

Many interesting features may be obtained from this analysis: (i) in the diffusive regime we have the important result that $\frac{\mathbf{D}_\beta^*}{D_\beta} = \frac{\mathbf{D}_{T\beta}^*}{D_{T\beta}}$ [25, 51], (ii) effect of pore-scale convection is complex and may lead to macro-scale thermodiffusion effects of opposite sign as shown in [25].

Most of the time, however, coupling is quite complicated and it is difficult to find a complete closure. This, of course, leaves the door open for the use of heuristic or semi-heuristic models, which is in fact the status of many models used in porous media physics. To illustrate this kind of problem, let us consider transport in porous media with intense phase change, like boiling occurring when cooling hot debris bed of nuclear reactor after a loss-of-coolant accident. So far, closures have been proposed in which the momentum transport is treated independently. Practical models make use of generalized Darcy's laws, or Forchheimer extensions [21, 37, 43]. These models remain largely heuristic and are not entirely supported by upscaling developments [5, 56, 71, 101], which in fact are made without taking into account the specifics of the phase repartition when boiling occurs in the porous medium. The need for non-equilibrium heat transfer model for Loca modelling has been recognized long ago [2, 14]. The macro-scale model has the form of a three-temperature model. A limited closure can be found for such a model assuming a quasi-static gas-liquid interface [33]. In this context, calculations of the effective properties suggested a significant difference between the values for a wet solid surface, so-called *slg* configuration, which would occur when boiling is not important, compared to a *sgl* configuration with a vapour film near the solid surface. Moreover, pore-scale nucleate boiling does not certainly fit with a quasi-static interface assumption! Therefore, it is expected that both two-phase and energy models should be impacted by the phase change process taking place within the pores. Experimental evidence interpreted through a three-temperature model [8] suggest that there is indeed an impact of the two-phase configuration on the effective properties and that, at least for the heat exchange coefficients, Nukiyama curves [68] specific to porous media configurations should be introduced.

5. CONCLUSIONS

The problem of heat transfer in porous media leads to several different classes of problems with more or less coupling between the mass, momentum and energy balance equations. Hence, the association of this diversity with the multi-scale aspect leads to various types of models, one to N-equations models of various mathematical forms, mixed or hybrid models. This multi-scale aspect has been the focus of this paper and these questions have been reviewed based on a classical heat transfer problem. It must be emphasized that strong non-linear coupled problems remain largely open questions and deserve further research.

It also must be remembered that several problems of paramount importance have not been addressed in this paper, in particular numerical modelling or the development of appropriate experimental techniques. Developments of new techniques in these area may offer new opportunities to understand and solve more and more of these multi-scale complex problems.

Nomenclature

Roman Symbols

\mathbf{b} mapping vector
 $\mathbf{n}_{\beta\sigma}$ normal vector

$\mathbf{w}_{\beta\sigma}$ interface velocity (m/s)
 a_v specific surface (1/m)
 c_p specific heat capacity (J/(kg.K))

c_β	mass fraction	Greek Symbols	
D_β	diffusion coefficient (m^2/s)	β, σ	Phase name
$D_{T\beta}$	Thermal diffusion coefficient, ($\text{m}^2/(\text{s.K})$)	ϵ	scale factor ($= l/L$)
k	thermal conductivity ($\text{W}/(\text{m.K})$)	Φ	homogeneous source term (W/m^3)
K_{eff}	effective thermal conductivity ($\text{W}/(\text{m.K})$)	ρ	density (kg/m^3)
L	macro-scale characteristic length (m)	ϵ	porosity
l	pore-scale characteristic length (m)	Ω	heterogeneous source term (W/m^2)
s	mapping scalar	Mathematical Symbols	
T	temperature (K)	$\langle \cdot \rangle$	volume average
U	intrinsic velocity (m/s)	$\langle \cdot \rangle^\alpha$	intrinsic volume average for the α -phase
V	averaging volume	\sim	deviation
v_β	pore-scale velocity (m/s)	$E(\cdot)$	expectation

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